National Center for Computational Sciences Snapshot
The Week of March 19, 2007

Salvaging Power from Exhaust

UNLV scientists team with GM to turn waste heat into electricity

As fuel prices rise, along with worries over pollution and global warming, scientists are looking at ways to make use of the heat that escapes from the tailpipes of our cars and trucks.

A team led by Changfeng Chen at the University of Nevada–Las Vegas is using the leadership computers at the National Center for Computational Sciences (NCCS) to investigate thermoelectric materials with the potential to route some of that energy back to the vehicle.

Chen's team is working with scientists from General Motors (GM) and Brookhaven National Laboratory to design materials that turn the heat into electricity that can then be used to recharge the vehicle's battery or power some of its systems. In particular, Chen and his team are using NCCS systems to perform first-principles simulations of the materials. Their simulations will be coordinated with experiments being done by a group at GM led by Jihui Yang and another at Brookhaven led by Qiang Li.

"We will be running simulations not just to support the experiments," Chen explained, "but to provide guidance for the materials as well."

The team has a 500,000-hour allocation on the center's Cray XT4 Jaguar system, and Chen made it clear he and his colleagues would like a long-term relationship with the NCCS.

"We're very happy that we have access to this state-of-the-art computer," he said. "Without access to this computer, we cannot run the calculations, period."

Former DOE Official Gil Weigand Joins ORNL HPC Management

Proven leader in the high-performance computing field brings years of experience to Oak Ridge National Laboratory (ORNL)

Former assistant energy secretary and Time Warner technology executive Gil Weigand has accepted a position with ORNL as director of strategic programs and planning with the Computing and Computational Sciences Directorate.

In this position Weigand will help develop new initiatives that integrate, consolidate, and focus the significant gains in computational-science capabilities on important global challenges related to energy, the environment, and national security. The planned

petascale and trans-petascale systems represent an unprecedented opportunity for science—one that will make it possible to use computation not only as a tool for explaining recognized phenomena, but also as a means of making fundamental discoveries and exploring the behavior of complex systems, including those involving humans.

Weigand served in several management positions with the Department of Energy (DOE) during the late 1990s and received the Secretary of Energy Gold Medal in 1996. Among the DOE titles he held were deputy assistant secretary for research, development, and simulation with the agency's Defense Programs, now National Nuclear Security Agency; deputy assistant secretary for strategic computing and simulation; and Defense Programs senior technical information officer.

During this time he oversaw one of the world's largest science-based research and development (R&D) programs and was responsible for managing an R&D budget of $2.2 billion focused on product invention and development in a range of science and computer disciplines key to nuclear-weapons simulation and technology.

Weigand was the architect behind DOE's highly successful Accelerated Strategic Computing Initiative. The program built a partnership between DOE laboratories and U.S. industry that developed the world's first supercomputer capable of a sustained performance of 1 trillion floating-point operations per second (1 teraflops). It also set the pace for the rapid advance in high-performance computing (HPC) that has led to current systems capable of hundreds of teraflops.

In the early 1990s Weigand held several positions within the Department of Defense. He served as director of the Modernization Office, where he headed the revitalization of HPC and networking at defense facilities, and as program director for high-performance computers at the Defense Advanced Research Projects Agency. As recognition for his work at DoD, he received the Secretary of Defense Medal for Outstanding Public Service in 1993.

After leaving DOE Weigand served as a media and technology executive at Time Warner, both in corporate positions and at the company's America Online (AOL) division. Weigand's positions with the company included vice president of the Corporate Technology Group as well as chief technology officer international and senior vice president for Web services at AOL.

Weigand's AOL group was responsible for several major product launches, including Netscape ISP and TotalTalk, a voice-over-internet-protocol service. While at Time Warner, Weigand remained personally active in R&D and holds 11 recent or pending patents in areas as varied as media restoration, streaming audio/video, and internet-protocol switching in cable-network head ends.

Weigand comes to ORNL from Canadian media giant CanWest, where he served as senior vice president for digital content at CanWest Media Works, Inc. In that position he

led the effort to create a company-wide enterprise to manage digital content and integrate business applications. He also managed initiatives for business-applications development and the advancement of a data center capable of supporting the company's broadcast, print, and internet businesses.

Weigand holds a doctorate in engineering from Purdue University.

Postdocs Like It

ORNL cited by magazine as a great place to work and learn

ORNL has cracked *The Scientist's* most recent list of "best places to work for postdocs." The Lab came in at No. 15 on the list of 15, and is the only national laboratory on the list.

The life sciences magazine's editor, Richard Gallagher, says, "Our survey is one of the few nationwide efforts to assess [postdoctoral students'] needs and desires and to recognize excellence in postdoc programs."

The Lab hosts from 200 to 250 postdocs. About 50 have assignments in the Computing for Computational Sciences Directorate, where many of them are converted to staff after serving in postdoctoral positions for one, two, or three years.

The survey covered 11 categories in which respondents judged their respective institutions. Categories included the quality of mentoring, the level of communication and opportunities for networking and career development. The magazine says most important factor cited was the quality of training and career preparation offered by an institution.

Also, UT-Battelle was been selected by *Training* magazine as a recipient of a "TOP 125" award honoring those companies that are "unsurpassed in harnessing human capital."

Oak Ridge High School Student Sponsored to New York Competition

Partnership with area high school is a "win" for both students and ORNL

Oak Ridge High School (ORHS) senior Sharice Brooks is getting a hand from Oak Ridge National Laboratory (ORNL) as she proves her business acumen at a competition in New York City.

Sharice, who has been working throughout the school year with the Computing and Computational Sciences Directorate, will be participating with her Virtual Enterprise class at ORHS in the Virtual Enterprise Trade Fair, which gives high school students an opportunity to learn the basics of business by marketing a fictional company.

Sharice received a check for $450 from Thomas Zacharia, ORNL's Associate Laboratory Director for Computing and Computational Sciences, to help with her expenses on the trip.

Her class will travel to New York in late March to compete with other students from around the world. The class will set up a trade-fair booth and will be competing in four areas: trade-fair booth, catalog design, Web design, and salesmanship.

The students' virtual business, known as Cynosure Telecom, markets cell phones and accessories. Sharice serves as the head of purchasing and sales. In that capacity she established the price for each of the firm's products by comparing the prices against both those of the company's virtual competitors and those of businesses in the real world.

Cynosure—the word means "something that guides" and is an alternate name for the North Star—hopes to sell $30,000 in virtual products out of the booth. The virtual company is an ongoing project at ORHS, with each class able to adjust the product line. This year, for instance, the students added accessories such as rhinestones, a global navigation system, ring tones, and prepaid minutes to the products for sale.

The trip won't be devoted entirely to work. While they are in New York, the students will also visit a number of traditional destinations, among them the Statue of Liberty and the Empire State Building. Sharice and the other students will see *The Phantom of the Opera* on Broadway. They will also visit the former site of the World Trade Center, which was destroyed in the terrorist attacks of September 2001.

Sharice's work with the directorate during the 2006–2007 school year has been through the Oak Ridge Business and Information Technology (ORBIT) Academy at ORHS. The academy allows ORHS students to work with businesses in the area while they pursue focuses in computer applications, Web design, computer repair, or finance.

Sharice has been an exemplary student, according to Linda Ousley, her teacher and coordinator for the ORBIT Academy at ORHS. "She is one you would like to clone," Ousley said. "She has a mature edge on her that a lot of teenagers don't have."

She has also been a great help to various Computing and Computational Sciences organizations during her 10-hour weeks, working with several mentors across the directorate. One such mentor, Sherry Hempfling of the User Assistance and Outreach Group at the National Center for Computational Sciences, is quick to sing her praises. "She's been invaluable here," Hempfling said. "She has a can-do attitude, and she's very quick to learn." For her efforts Sharice received an A+ in her work-experience class, a grade Hempfling says is well deserved.

Once she graduates from ORHS, Sharice plans to enroll in ITT Technical Institute in Knoxville, where she will pursue an associate's degree in multimedia studies. She expects to eventually earn a bachelor's degree in graphic design.